Diffusion Enhances Chirality Selection

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Diffusion effect on chirality selection in a two-dimensional reaction-diffusion model is studied by the Monte Carlo simulation. The model consists of achiral reactants A which turn into either of the chiral products, R or S, in a solvent of chemically inactive vacancies V. The reaction contains the nonlinear autocatalysis as well as recycling process, and the chiral symmetry breaking is monitored by an enantiomeric excess ϕ.

Without dilution a strong nonlinear autocatalysis ensures chiral symmetry breaking. By dilution, the chiral order ϕ decreases, and the racemic state is recovered below the critical concentration c_c. Diffusion effectively enhances the concentration of chiral species, and c_c decreases as the diffusion coefficient D increases. The relation between ϕ and c for a system with a finite D fits rather well to an interpolation formula between the diffusionless($D = 0$) and homogeneous ($D = \infty$) limits.

I. INTRODUCTION

It has long been known that natural biomolecules choose one type of enantiomer among the two possible stereostructures, and the chiral symmetry is broken in life: Amino acids in proteins are all L-type, while sugars in nucleic acids are all D-type [1, 2, 3]. There are many studies on the origin of this homochirality, but the asymmetry caused by various proposed mechanisms turned out to be very minute [4, 5, 6]. Frank found more than fifty years ago that a linear autocatalysis accompanied by mutual inhibition are necessary in an open system for the amplification of enantiomeric excess (ee) of one type [7]. The model with enantiomeric cross-inhibition is extended to polymerization models [8, 9]. Experimental realization of the ee amplification is found recently in pyrimidyl alkanol [10], and explained by a nonlinear autocatalytic process in a closed system [11, 12]. Addition of a recycling process to this nonlinear system is shown to realize an asymptotic selection of a unique chiral state [13]. The importance of recycling process is also shown in nonautocatalytic but a polymerization-epimerization model [14].

All the above arguements assume that the reaction takes place homogeneously. For spatially extended systems, however, the inhomogeneity affects symmetry breaking in general. In condensed matter systems, for instance, elements are located densely in contact with each other, and interactions propagate through neigboring elements so as to cause coherent phase transitions. In contrast to the equilibrium symmetry breaking in the condensed matter, organic molecules in the primordial era might have been distributed dilutely in a solution. If this were the case, molecular transport is necessary in order to bring molecules come into contact to activate

autocatalysis.

In a previous letter[15] we briefly reported the diffusion effect on the chiral symmetry breaking. Here we give a more detailed work of the diffusion effect on the chirality proliferation in an extended system. After introducing the model and Monte Carlo simulation algorithm in §2, we consider first the chirality selection in a diffusionless system, and point out some similarity of the present chemical reaction system to the Ising ferromagnet in §3. There, the effect of site dilution is also discussed. In §4, the diffusion effect is studied systematically and the chiral symmetry breaking is found to be enhanced by the diffusion. It is qualitatively interpreted that the diffusion effectively increases the concentrations of chemically active molecules, and consequently promotes autocatalysis. The idea is summarized in a simple interpolation formula as for the diffusion coefficient dependence of the order parameter and the concentration relation. The study is summarized in §5.

II. MODEL AND SIMULATION ALGORITHMS

The model we study is essentially the same with the one proposed in a previous letter [15]. There are four types of molecules; an achiral reactant A, two types of product enantiomers R and S, and a solvent molecule in a diluted system, which we call a vacancy V. Molecules are treated as entities which occupy square lattice sites and can move randomly thereon. Double occupancy of a lattice site is forbidden.

Various processes in the system are summarized in Fig.1. An isolated achiral reactant A turns into a chiral R or S molecule with a rate k_0, as in Fig.1(a). When there is one R(S) molecule in the nearest neighbor of a reactant A, the production rate of R(S) increases by an additional linear autocatalytic rate k_1, as in Fig.1(b). When there are two or more R's(S's) in the nearest neighborhood, the production rate of R(S) is further enhanced by an additional nonlinear autocatalytic rate k_2, as in Fig.1(c).

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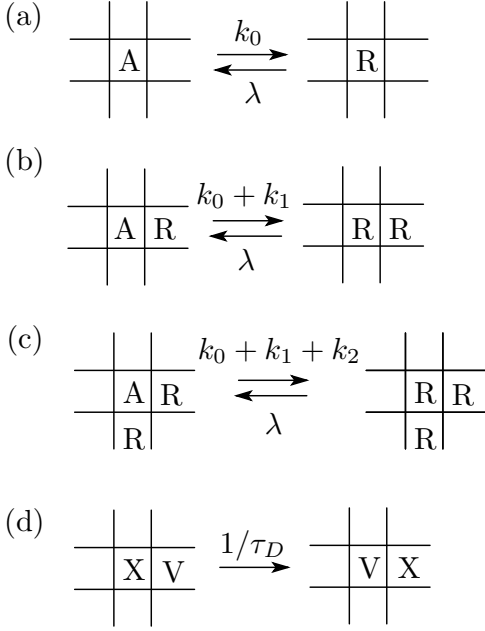†Electronic address: hyuga@rk.phys.keio.ac.jp

FIG. 1: Various processes with transition probabilities; (a) non-autocatalytic, (b) linearly autocatalytic, (c) nonlinearly autocatalytic reactions with recycling and (d) a vacancy diffusion. X in the diffusion process (d) represents chemically active species, A, R or S.

The rate of back reaction λ is assumed constant, independent of the environment around chiral molecules, R or S (Fig.1(a)-(c)). By these chemical reaction processes, the number densities a, r and s of active molecules A, R and S vary, but the total number density of active molecules $a+r+s=c$ is fixed constant, reflecting the assumption of a closed system corresponding to the Soai reaction [10]. The degree of chiral symmetry breaking is represented by the enantiomeric excess (ee) order parameter

$$\phi = \frac{r-s}{r+s}. \tag{1}$$

A vacancy V is inactive as for the chemical reaction, but plays a vital role in the diffusion process. When chemically active species, A, R and S, are neighboring to V, they exchange their sites with V randomly with a life time τ_D on average, as in Fig.1(d). The diffusion coefficient is then $D = a^2/(4\tau_D)$ with a being the lattice constant and set to be unity hereafter. Previously we simulated only the case with $D = 1/4$, because the Metropolis algorithm was used in the Monte Carlo simulation [15]. In the present paper we want a systematic study of diffusion effect on the chirality selection, and therefore an arbitrary variation of the diffusion coefficient D is necessary. For that purpose, we adopt a waiting time algorithm for the Monte Carlo simulation.

The simulation runs as follows: All the positions which can undertake a process i are tabulated in a list; every site

in the list has the same transition probablity P_i to perform the reaction or diffusion process i, shown in Fig.1. Assume that there are n_i lattice sites in the corresponding list of the process i. Then, the total probability of events in a unit time is obtained as $P_{\text{tot}} = \sum_i P_i n_i$. In other words, in a time interval $dt = 1/P_{\text{tot}}$, one of the process takes place on average. By generating a quasi-random number x which is uniformly distributed between 0 and P_{tot}, the process j which satisfies the condition

$$\sum_{i=1}^{j-1} P_i n_i \leq x < \sum_{i=1}^{j} P_i n_i \tag{2}$$

is to be performed. The lattice site which performs the process j is listed at the k-th position in the list of n_j sites, where $y = x - \sum_{i=1}^{j-1} P_i n_i$ and k is the integer part of $y/P_j + 1$ as

$$k = \left[\frac{y}{P_j} + 1\right]. \tag{3}$$

After performing the process j on the site in the k-th position in the list, the time is advanced by dt and the lists are updated. We simulate systems with sizes 50^2 and 100^2, but in the following we show results obtained for the larger system with a size 100^2.

III. WITHOUT DIFFUSION

From our previous works on a homogeneous system [13, 15] the nonlinear autocatalysis with a finte k_2 is found essential for the chiral symmetry breaking, whereas the linear autocatalysis k_1 is inefficient. Therefore, k_1 is set absent hereafter: $k_1 = 0$. In order to find out the effect of diffusion, we consider in this section the developement of chirality in space without the material transport. The effect of diffusion is studied in the next section. Here, the order of chiral symmetry breaking is studied as a function of the strength of the nonlinear autocatalysis or of the concentration of active molecular species.

A. Chiral Symmetry Breaking as a function of Nonlinear Autocatalysis

First, we consider the k_2-dependence of the chiral symmetry breaking, when the whole lattice sites are occupied by chemically active species; $c = 1$. When the nonlinear autocatalytic effect is strong enough such as $k_2 = 100k_0$ with $\lambda = k_0$, achiral reactant A quickly reduces to chiral species R or S. Therefore, even by starting from an achiral initial configuration with only achiral reactants A, domains of R and S are formed in the early stage, as shown at a time $k_0 t = 50$ in Fig.1. Then, the domain competition sets in, and those domains surrounded by another type shrink as shown in the middle column in Fig.2. Eventually, competition ends up by the dominance
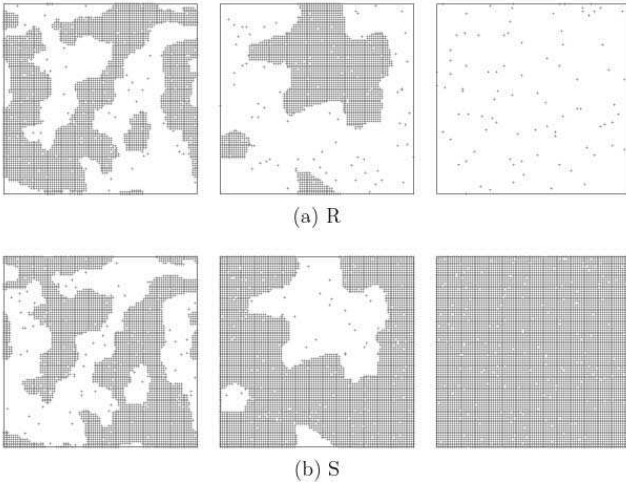
(a) R

(b) S

FIG. 2: Configuration evolution of (a) R and (b) S molecules in a diffusionless system. Tmes are $k_0 t = 50, 250, 1750$ from left to right. Parameters are $k_0 = \lambda$, $k_1 = 0$, $k_2 = 100 k_0$ with $c = 1$, and the system size is 100^2.
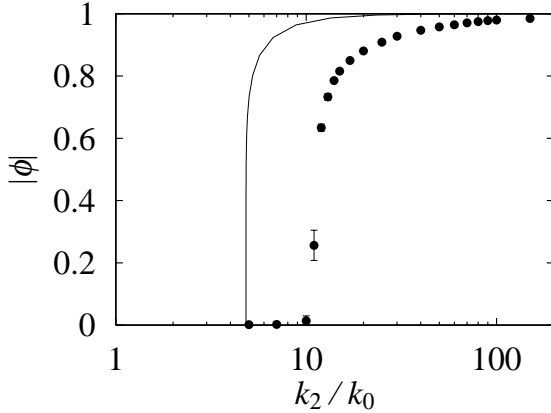

FIG. 3: Enantiomeric excess $|\phi|$ versus k_2/k_0 at the full occupation $c = 1$ in a semi-logarithmic plot. A curve represents the temperature dependence of the magnetization [20] of a square Ising model, where a temperature is related to the chemical reaction rates as $k_2/k_0 = \exp(4J/k_B T) - 1$.

of one enantiomeric type, S in the case shown in the right column of Fig.2. In some cases the system decouples into two inter-penetrating domains of R and S, both of which in effect extend to infinity due to the periodic boundary conditions in the x and y directions: Then, it takes an enormous time until the minor domain extinguishes and the system accomplishes the final equilibrium state.

In order to obtain the equilibrium value of the order parameter ϕ in a reasonable simulation time, therefore, we start simulations from an initial configuration such that the whole lattice sites are occupied by R species. Equilibrium states are readily realized from this initial
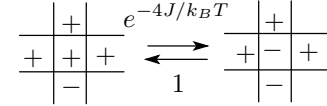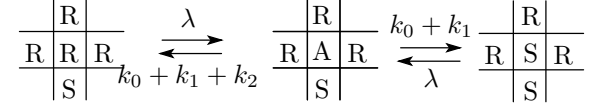
(a)
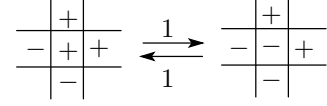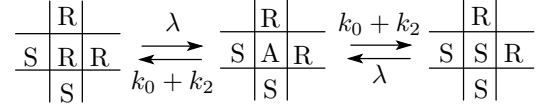
(b)

FIG. 4: Analogies of state transition in the reaction model (above) and the Ising ferromagnet (below). (a) $n = 2$, and (b) $n = 3$.

configuration, and the equiblirium value of the order parameter ϕ thus obtained is shown in Fig.3 at various strength of nonlinear autocatalysis k_2/k_0. Since the non-autocatalytic reaction k_0 drives the system to the racemic state, the value of the order parameter ϕ decreases as k_2 decreases, and vanishes at a critical value of k_2/k_0 around 10: The system recovers the chiral symmetry, getting into the racemic state.

The qualitative features of domain competition shown in Fig.2 and the emergence of symmetry breaking at large k_2 as shown in Fig.3 suggest us some resemblance with the phase transition in an Ising ferromagnet. In fact, one may find some analogy of our reaction system to an Ising ferromagnet: In the latter, each lattice site is occupied by an Ising spin, which can be in one of the two states; up or down. When a nearest neighboring spin pair have the same orientation, the energy is low as given by $-J < 0$, whereare when a pair is in opposite orientations, the energy is high as $J > 0$: The energy difference is set to be $2J > 0$. At a temperature T, a spin flips its orientation with a transition probability which depends on the associated energy change. Let the spin to flip have n nearest neighboring spins with the same orientation. Then, it will have $4 - n$ spins of the same orientation after the flip, and we denote the transition probability as $W(n \rightarrow 4 - n)$. In order to ensure thermal equilibrium asymptotically, it is known to be sufficient if the detailed balance condition between the transition probabilities of

one process and its reverse

$$\frac{W(n \to 4-n)}{W(4-n \to n)} = \exp(-\Delta E/k_B T) \quad (4)$$

is satisfied, where $\Delta E = 4(n-2)J$ represents an energy change. For example, when a site is surrounded by two up spins and two down spins, $n = 2$ and the transition probability of an up spin to flip downward is equal to its reverse process, as shown in the lower column of Fig.4(a). Then, in equilibrium the probabilty $P_+(2,2)$ of an up spin surrounded by two up spins and two down ones is equal to that of a down spin in the same enviornment $P_-(2,2)$: $P_+(2,2) = P_-(2,2)$. We associate, for instance, R and S molecules to the up and down Ising spins, respectively. Then, the transitions for $n = 2$ in the Ising model correspond to transitions between an R and S molecule surrounded in the neighborhood by two R's and two S's (upper column of Fig.4(a)). Since the alternation of R and S is mediated by an achiral reactant A, the equilibrium probabilities of R and S in the configuration Fig.4(a) are related as $\lambda P_R(2,2) = (k_0+k_2)P_A(2,2) = \lambda P_S(2,2)$, and thus $P_R(2,2) = P_S(2,2)$, consistent with our assignment of R and S molecules to up and down spins. When a site is surrounded by three R's and one S molecule as in the upper column of Fig.4(b), the equilibrium probability that the site is occupied by an R molecule $P_R(3,1)$ is higher than the one by an S molecule $P_S(3,1)$. They are related as $\lambda P_R(3,1) = (k_0+k_2)P_A(3,1)$ and $k_0 P_A(3,1) = \lambda P_S(3,1)$, and thus $P_R(3,1) = (1+k_2/k_0)P_S(3,1)$: At a lattice site surrounded by three R's and an S, the probability of finding an R molecule is higher than that of finding an S molecules by a factor $(1+k_2/k_0)$. For the Ising system, the corresponding situation is the spin on the site surrounded by three up's and one down; $n = 3$. The relation between probabilities that a site is occupied by an up spin and by a down is $e^{-4J/k_B T}P_+(3,1) = P_-(3,1)$. Thus, we may assume that the ratio $(1 + k_2/k_0)$ corresponds in the Ising model to the ratio of the transition probabilities $\exp(4J/k_B T)$. (See the lower column of Fig.4(b)). In other word, the nonlinear autocatalytic rate k_2 in our chiral model might correspond to the coupling constant of the two-dimensional Ising model as

$$k_2/k_0 = e^{4J/k_B T} - 1. \quad (5)$$

Since the numbers of R and S molecules correspond to those of up and down spins in the Ising ferromagnet, the chiral order parameter ϕ corresponds to the spontaneous magnetization M of the Ising model. The latter is exactly known to behave as [20] $M = [1 - \sinh(2J/k_B T)^{-4}]^{1/8}$. By using the relation (5), the magnetization M is plotted in Fig.3 by a continuous curve.

The transition temperature T_c of the Ising model on the square lattice is exactly known to be at $k_B T_c/2J = 1/\ln(1+\sqrt{2}) \approx 1.135$. Thus in the present reaction model the chiral symmetry breaking is expected to take place at $k_2 \geq k_{2c} = 2(\sqrt{2}+1)k_0 \approx 4.83k_0$. However, the order parameter ϕ obtained by simulations decreases faster than

the Ising magnetization as k_2 decreases: For the chiral symmetry breaking a larger value of the nonlinear auto-catalysis $k_2 \approx 10k_0$ is required, as shown in Fig.3. This is because of the approximate character of the relation between the Ising coupling constant J and the nonlinear autocatalytic rate k_2. The production rate in our model is independent of the number of neighboring R(S) species as far as it is more than 2, whereas transition rate to the up spin state in an Ising model increases as the neighboring number of up spins increases: This means that our coupling constant k_2 is effectively weaker than the Ising coupling parameter. Also the existence of an achiral species is not included in the Ising model. The decomposition process from a chiral species R or S back to an achiral reactant A induces fluctuation which breaks ordering, and a chirally ordered state in our reaction model is less stable than the ferromagnetic state in the Ising ferromagnet: The strong nonlinearity is necessary for the symmetry breaking. In fact, the critical value for the chiral symmetry breaking k_{2c} depends on the decomposition rate λ, though the k_2 versus J relation in eq.(5) is independent of λ. From simulations with a large $\lambda = 10k_0$, the order is found to be easily broken at $k_{2c} \approx 23k_0$, whereas for small $\lambda = 0.1k_0$ the order holds until $k_{2c} \approx 9k_0$.

B. Dilution Effect on Chiral Symmetry Breaking

We now keep the nonlinear autocatalitic effect as strong as $k_2/k_0 = 100$, and consider the dilution effect $(c < 1)$ on the chiral symmetry breaking. If there is no material transport, the behavior of the system depends strongly on the arrangement of vacant sites. Therefore, in order to obtain the order parameter ϕ we average 9 samples at concentrations lower than $c = 0.7$, whereas 3 samples seem sufficient at higher concentrations. As the system is diluted, the probability that active chemical species are contiguous to each other decreases. In the present reaction model, however, a reactant A should be surrounded by chiral products R or S to sustain the autocatalysis. Therefore, the chiral symmetry breaking is possible only at concentrations at least larger than the site percolation threshold of the square lattice $c_p = 0.592746$ [16, 17]. Below c_p, the information of one site is unable to propagate through the whole system, and thus the system cannot be in a single state. The order parameter ϕ actually decreases as the system is diluted, as shown in Fig.5a, and the system becomes racemic at concentrations lower than the critical value $c_c(D = 0)$. By assuming a critical concentration at $c_c(D = 0) \approx 0.639$, the order parameter ϕ shows a power-law dependence $\phi \propto \sqrt{c - c_c(D = 0)}$, as shown in Fig.5(b). The critical concentration $c_c(D = 0)$ without diffusion is close to but larger than c_p.

A rather large discrepancy between $c_c(D = 0)$ and c_p might be understood by using the similarity of the present diluted reaction model to a site-diluted Ising fer-

romagnet, where lattice sites are diluted substitutionally by nonmagnetic impurities [18]. In a site-diluted Ising model, the transition temperature is known to decrease as the concentration of nonmagnetic impurity increases, and the phase transition vanishes at the critical concentration close to the percolation threshold c_p [19]: The transition temperature is zero at the critical concentration. If the relation (5) holds, however, our reaction model with $k_2 = 100k_0$ corresponds to an Ising ferromagnet at a finite temperature $k_B T/2J = 0.433$ or $T/T_c = 0.38$. A thermal fluctuation favors the recovery of the symmetry even if a percolating cluster exists, and this may be the reason that the critical concentration $c_c(D = 0)$ is larger than the percolation threshold c_p.
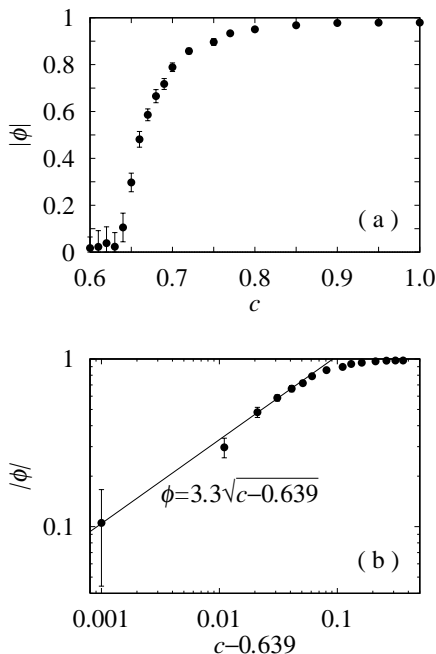

FIG. 5: Enantiomeric excess $|\phi|$ versus c in a diffusuioness system with a strong nonlinear autocatalysis $k_2/k_0 = 100$.

IV. DIFFUSION ENHANCEMENT OF THE CHIRALITY SELECTION

We now study the diffusion effect on the chirality selection in a diluted system. The transport of material in general increases the chance for an achiral reactant A to meet chiral products R and S in their lifetimes, and may enhance the autocatalytic effect. When the diffusion is extremely fast, the system becomes homogeneous: This case will be studied in the following subsection analytically. With a finite diffusion coefficient, numerical simulation is the only possible method to study, and the results so obtained will be analyzed by the interpolation formula in the second subsection.

A. Homogeneous Case with $D = \infty$

When the diffusion is extremely fast, the system becomes homogeneous. Then, the simple mean field approximation leads to the rate equations for the homogeneous concentrations;

$$\dot{r} = k(r)a - \lambda r$$
$$\dot{s} = k(s)a - \lambda s, \quad (6)$$

with the rate constant $k(r) = k_0 + 4k_1 r + 6k_2 r^2$. Here in this subsection we restore the rate k_1 of the linear autocatalytic reaction, in order to be general. The factors $4r$ and $6r^2$ represent the probabilities that at least one or two of the four neighboring sites are occupied by R species, respectively, in the sense of mean field approximation. Since the system is assumed to be closed, the total concentration of chemically active species satisfies the concervation law; $a + r + s = c =$ const. Then, the total concentration of chiral products $u = r + s$ is shown to varies as

$$\dot{u} = [2k_0 + 4k_1 u + 3k_2 u^2(1 + \phi^2)](c - u) - \lambda u, \quad (7)$$

whereas the order parameter ϕ evolves as

$$\dot{\phi} = \frac{c - u}{u} \phi[-2k_0 + 3k_2 u^2(1 - \phi^2)]. \quad (8)$$

Since $0 \leq u \leq c$, eq.(8) is similar to the time-dependent Landau equation with nontrivial fixed points if $u^2 > 2k_0/(3k_2)$. The other point to remark is that eq.(8) does not depend explicitly on the linear autocatalytic rate k_1; ϕ depends on k_1 only implicitly through u. Thus the linear autocatalysis alone cannot break the chiral symmetry.

The equilibrium values of u and ϕ are calculated from the algebraic equations given by $\dot{\phi} = \dot{u} = 0$. The spontaneous chiral symmetry breaking takes place at a critical concentration $c_c(D = \infty)$ when the diffusion is infinitely fast: The order parameter ϕ of a homogeneous system takes a finite value for $c_c(D = \infty) < c \leq 1$. For $k_1 = 0$ the order parameter ϕ is explicitly written as a function of the concentration c as

$$\phi^2 = 1 - \frac{6k_0 k_2}{\lambda^2}\left(c - \sqrt{c^2 - \frac{2\lambda}{3k_2}}\right)^2, \quad (9)$$

and the critical concentration is calculated to be $c_c(D = \infty) = (4 + \lambda/k_0)/\sqrt{k_0/24k_2}$. It takes the value $c_c(D = \infty) = 0.1020$ for the parameter values $k_1 = 0$, $k_2 = 100k_0$, $\lambda = k_0$.

B. Finite Diffusion Constant

The emergence of chiral order at a finite vacancy diffusion is studied by the Monte Carlo simulation. It is found that the symmetry breaking takes place rather rapidly
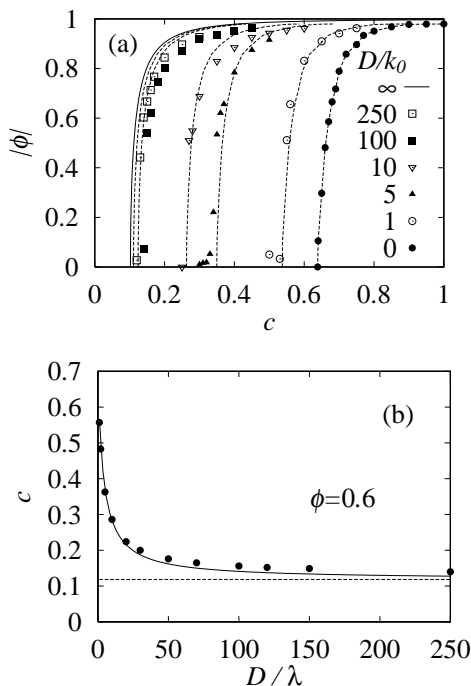
FIG. 6: (a) Enantiomeric excess $|\phi|$ versus c at various values of the diffusion coefficient D/k_0. The reaction parameters are $k_2/k_0 = 100$, $k_1 = 0$ and $\lambda = k_0$. A continuous curve represents the relation (9) for a homogeneous system. Dashed curves represent interpolation (10) at various diffusion coefficients. (b) Diffusion coefficient dependence of the concentration c where the order parameter takes the value $\phi = 0.6$. A curve represents the interpolation (10) with a parameter $A = 0.235$. The dotted line represents the homogeneous case with $c(0.6; D = \infty) = 0.118$.

even if we start from a completely achiral initial configuration with all the chemically active molecules being achiral reactant A as $a = c$: The order parameter approaches quickly the asymptotic value, though which enantiomer dominates over the other is determined randomly in each simulation run. Therefore, we initiated the simulation from the complete achiral state with only A and V species.

The steady-state value of ee or $|\phi|$ at various values of diffusion coefficient D is shown as a function of the concentration of active species c by symbols in Fig.6(a). A continuous curve represents the relation (9) for a homogeneous system with $D = \infty$. The most striking feature is that $\phi - c$ relations at different D's look similar but with shifts to the lower concentration as D increases. The D-dependence of the shift might be considered in the following way. The chiral products R or S once produced diffuse around in a diffusion area of about D/λ sites during the life time λ. Therefore, in a system where diffusion is allowed the effective density of chiral catalysts is enhanced by a factor $1 + AD/\lambda$ in comparison to the system without diffusion. A proportionality constant

A will be determined later by fitting to the simulation results. With a very large diffusion D, however, there will be overlappings of various diffusion areas, and the diffusive enhancement may saturate. Thus, even with an infinitely fast diffusion, a finite concentration of active species is necessary, as is given by eq.(9).

The diffusive enhancement of the effective concentration means that in order to reach a fixed value of the order parameter ϕ, the required concentration of active species $c(\phi; D)$ for a system with a finite diffusion coefficient D can be less than $c(\phi; D = 0)$ for a diffusionless system. Here we propose a simple formula for $c(\phi; D)$ interpolating between the diffusionless limit $c(\phi; D = 0)$ and the homogeneous limit $c(\phi; D = \infty)$ as

$$c(\phi; D) = \frac{c(\phi; 0) + c(\phi; \infty)(AD/\lambda)}{1 + (AD/\lambda)}, \qquad (10)$$

where $c(\phi; 0)$ is obtained by the simulation (Fig.5(a)), whereas $c(\phi; \infty)$ is obtained by solving eq.(9) as

$$c(\phi; \infty) = \frac{1}{\sqrt{24k_0 k_2}} \Big(\lambda\sqrt{1 - \phi^2} + \frac{4k_0}{\sqrt{1 - \phi^2}} \Big). \qquad (11)$$

To determine the constant A, we fit the formula (10) with simulation data at $\phi = 0.6$. The reason for the choice of a non-zero value of ϕ is that the value of $c(\phi; D)$ is expected to be more accurate away from the transition point, $\phi = 0$. The fit gives the value $A \approx 0.235$, and agrees well at small D but deviates systematically at large D, as shown in Fig.6(b).

With this value of A, we interpolate the whole $\phi - c$ curve for arbitrary D by eq.(10), as is drawn by broken curves in Fig.6(a). The trend of the down shifting in the concentration as the diffusion increases is well reproduced, even though the fitting is not perfect, especially at a large diffusion coefficient D. There, we have so far no plausible theory on the D-dependence of $c(\phi; D)$.

V. SUMMARY AND DISCUSSIONS

We study diffusion effect on the chirality selection during a chemical production of chiral molecules, R or S, from an achiral substrate A in a solution by means of a square lattice model. In addition to the usual reactions of the production and the decompsition of chiral species, autocatalytic processes are incorporated such that an achiral substrate surrounded by many enantiomers of one type increases the turn-over rate to that type. Specifically, the nonlinear autocatalysis which takes place when the substrate is surrounded by two or more enantiomers of one type is found to be essential in the chiral symmetry breaking.

When all the lattice sites are ocuupied by chemically active species, A, R or S, the spontaneous symmetry breaking has some similarity to the phase transition of an Ising ferromagnet. The strength of the nonlinear autocatalysis k_2 in our chemical model is approximately related to the Ising coupling constant. The chemical model

at very large k_2 evolves through the domain competition, similar to the dynamics of the Ising model at low temperatures. As k_2 decreases, the chiral order extinguishes, but earlier than the expectation from the Ising model. The discrepancy may be due to the larger degrees of freedom; three in the chemical model whereas two in the Ising model.

Inclusion of vacancies or dilution suppresses the degree of the chiral symmetry breaking or the enantiomeric excess ϕ, and below the critical concentration of chemically active species, the system is in a racemic state with a chiral symmetry. In a diffusionless system ($D = 0$) with a strong nonautocatalysis, the system is similar to the site-diluted Ising model, and the critical concentration is close to but larger than the percolation threshold c_p.

Diffusion enhances the chiral order ϕ, since the migration of chiral products enhances the chance of molecular collision and the autocatalytic process as well. In the limit of an infinitely fast diffusion ($D = \infty$), the system behaves as if it is homogeneous and the rate equation in the mean field approximation describes the chiral symmetry breaking: The steady state solution is obtained analytically in this limit. At a finite diffusion coefficient D, the concentration dependence of ϕ is shifted from the diffusionless limit ($D = 0$) to the homogeneous limit ($D = \infty$). The behavior is interpreted as the diffusive enhancement of concentrations of chiral species, and is summarized in an interpolation formula of c-dependence of ϕ or $c(\phi; D)$ between the two limits.

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